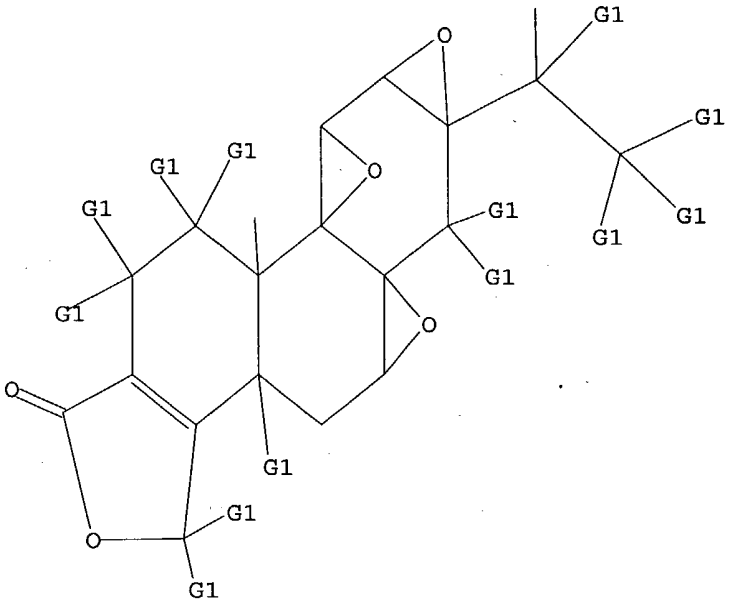
9/27/2004

STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 H,O,F,CF2,CF3,OH

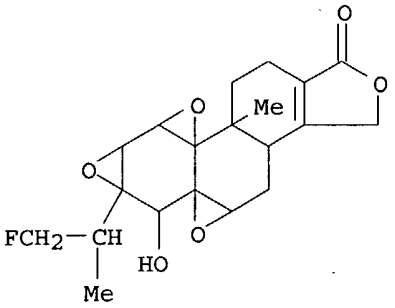
s l5 and fluoro
2489681 FLUORO
15 FLUOROS
2489681 FLUORO
(FLUORO OR FLUOROS)
L8 1 L5 AND FLUORO

=> d l8 iall

L8 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 139601-52-8 REGISTRY
ED Entered STN: 13 Mar 1992
CN **Triptolide, 16-fluoro- (9CI)** (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN **Trisoxireno[4b,5:6,7:8a,9]phenanthro[1,2-c]furan, triptolide deriv.**
MF C20 H23 F O6
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C2O-C2O-C2O- C4O-C6-C6-C6	OC2-OC2-OC2- OC4-C6-C6-C6	3-3-3-5-6-6- 6	C16O4	6372.1.1	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	3.20	pH 1	(1) ACD
Bioconc. Factor (BCF)	3.20	pH 4	(1) ACD
Bioconc. Factor (BCF)	3.20	pH 7	(1) ACD
Bioconc. Factor (BCF)	3.20	pH 8	(1) ACD
Bioconc. Factor (BCF)	3.20	pH 10	(1) ACD
Boiling Point (BP)	622.2+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	105.67+/-6.0 kJ/mol		(1) ACD
Flash Point (FP)	330.1+/-56.7 deg C		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	80.0	pH 1	(1) ACD
Koc (KOC)	80.0	pH 4	(1) ACD
Koc (KOC)	80.0	pH 7	(1) ACD
Koc (KOC)	80.0	pH 8	(1) ACD
Koc (KOC)	80.0	pH 10	(1) ACD
logD (LOGD)	0.97	pH 1	(1) ACD
logD (LOGD)	0.97	pH 4	(1) ACD
logD (LOGD)	0.97	pH 7	(1) ACD
logD (LOGD)	0.97	pH 8	(1) ACD
logD (LOGD)	0.97	pH 10	(1) ACD
logP (LOGP)	0.968+/-0.754		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	378.39		(1) ACD
Vapor Pressure (VP)	4.37E-18 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.67 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

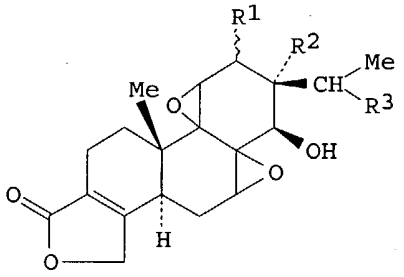
REFERENCE 1

ACCESSION NUMBER: 116:136234 CA
TITLE: Isolation of 17-hydroxytriptolide and analogs as drugs

INVENTOR(S): Ma, Pengcheng; Zheng, Jiarun; Lu, Xieyu
PATENT ASSIGNEE(S): Chinese Academy of Medical Sciences, Institute of Skin Disease, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 12 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
INT. PATENT CLASSIF.:
MAIN: C07D493-22
CLASSIFICATION: 63-4 (Pharmaceuticals)
Section cross-reference(s): 30
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1052859	A	19910710	CN 1989-105432	19891222
US 5430054	A	19950704	US 1990-629411	19901218
PRIORITY APPLN. INFO.:			CN 1989-105432	19891222
			CN 1989-105433	19891222
			CN 1989-105434	19891222
			CN 1990-105750	19901013

GRAPHIC IMAGE:



I

ABSTRACT:
The title compds. (I; R1 = halo, OH, MeO; R2 = F, Cl, OH, R1R2 = O; R3 = halomethyl, CH2OH, CH2OMe, CHO, etc.), useful as antiinflammatory, antitumor, contraceptive agents, and immunosuppressants (no data), are isolated from Tripterygium wilfordii. Extraction of 20 kg T. wilfordii with 75-95% EtOH, concentration,
partition in CHCl3, and silica gel column chromatog. gave pure triptolide (I: R1R2 = O; R3 = CH2OH), which was hydrolyzed with HX (X = halo) to give I (R1 = X, R2 = OH, R3 = CH2OH) and further reacted to give addnl. I derivs.

SUPPL. TERM: hydroxytriptolide isolation Tripterygium; triptolide analog isolation Tripterygium
INDEX TERM: Tripterygium wilfordii
(hydroxytriptolide analogs isolation from)
INDEX TERM: 139713-80-7
ROLE: PROC (Process)
(isolation of, from Tripterygium wilfordii)
INDEX TERM: 139601-39-1P 139601-40-4P 139601-41-5P 139601-42-6P
139601-43-7P 139601-44-8P 139601-45-9P 139601-46-0P
139601-47-1P, Triptolid-16-oic acid 139601-48-2P
139601-49-3P 139601-50-6P 139601-51-7P 139601-52-8P
139601-53-9P 139601-54-0P
ROLE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use);